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HEAD PISTON GEOMETRY OPTIMIZATION: A CRFD STUDY APPLIED TO A LOCOMOTIVE ENGINE

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Abstract. *Daily people make use of different kinds of transport, in turn, its powertrain systems are mostly provided with internal combustion engines using, usually, fossil fuels. Along the last years these engines have been modernized and have become more efficient and less polluting, however, fuel consumption and emissions still as the more critical points for the engine operation. In this way, studies of sustainability, energy efficiency and optimization of existing internal combustion engines are extremely necessary to obtain efficiency improvements by reducing the fuel consumption and pollutants to allow the continuity of use of these engines until they can be replaced. The rail transport sector is used worldwide for the transport of passengers as well as for the transport of cargo, using powerful internal combustion engines and consequently large consumers of fuels such as diesel. Studies to optimize these engines are necessary so that they become more efficient and less polluting. By optimizing the injection system parameters such as the fuel spray angle, or piston head geometry, for example, it is possible to obtain an efficiency gain. This work focuses on the piston head geometry optimization of a diesel-powered railway internal combustion engine through numerical analysis. For this, the AVL-FIRE™ software was used. The engine optimization was performed using the following variables: in-bowl radius, top dead center clearance gap and top bowl center depth. The results are then analyzed in terms of power, torque, fuel consumption and emissions giving around 2.88% higher IMEP, 2.18% higher power and torque and 2.78% less specific fuel consumption when compared to the base engine geometry.*

Keywords: *Rail Diesel Engine, Computational Reactive Fluid Dynamics (CRFD), Optimization, AVL-FIRE™ , Piston Head Geometry*

1. INTRODUCTION

The transport sector is responsible for a considerable portion of the emission of pollutants, since this sector uses mostly large internal combustion engines and powered by diesel (Abdel-Rahman, 1998). Among these sectors, the railway sector stands out because, in general, trains move large loads and for that, large engines are needed (Hoseini *et al.*, 2017). Therefore, studies to make these engines more efficient are extremely necessary and important. As they are large engines, they consume significant amounts of fuel while emitting large amounts of polluting gases such as NO and soot (Rymaniak *et al.*, 2019).

In a study carried before by this research group (Henschel Jr. and Cancino, 2019), it was verified that when changing the injection angle from 160° to 153° in a General Electric model GE 7FDL railway engine through numerical simulation of computational reactive fluid dynamics (CRFD) using the AVL FIRE™ ESE Diesel tool, it was possible to obtain gains in terms of power and torque for this engine, as well as reducing the specific consumption of fuel. In this sense, this study has the intention to continue the study carried out previously. Therefore, the piston head geometry optimization will be performed using the AVL FIRE™ DVI (Design Variation Interface - Design of Experiments and Optimization) tool in order to obtain the best IMEP (indicated mean effective pressure). With the optimized piston head geometry, engine simulations using the remodeled engine piston geometry (the optimized one) were then carried out, obtaining gains in terms of power and torque for engine. The study also aims to analyze emissions and fuel consumption so that the performance of this engine is more efficient and finally to compare the results with the original engine and also with the engine simulated by Henschel Jr. and Cancino (2019).

2. RAIL ENGINES LITERATURE REVIEW

The rail transport sector is a representative consumer of fossil fuels because of large internal combustion engines are needed to transport large amounts of cargo. This consumption represents a big part of the costs involved in this kind of transport (Pereira, 2009). In this way, a gain in efficiency and a reduction in fuel consumption of these engines is of great significance. Several studies carried out to obtain performance gains are developed in this sense, either through changes in the fuel injection angle (Soni and Gupta, 2017), or even on the effects that changing the injection angle can promote (Wei *et al.*, 2014), as well as the effects of changing the system geometry. In addition, studies on how the influence of injection strategies influence emissions in diesel engines (Gorji-Bandpy *et al.*, 2009) and also on how these emissions can be minimized with the optimization of injection systems (Soni and Gupta, 2017) are essential to reduce the amount of gases emitted into the atmosphere. However, these studies depend on making physical changes in these engines, which often requires high costs to carry out the changes and research, in this sense the realization of studies through numerical CFD/CRFD simulations (Reitz and Rutland, 1995) can represent significant savings and enable future projects.

2.1 The engine operation of CI-ICE and piston head geometry optimization

Compression ignition internal combustion engines (CI-ICE) are used in vehicles that require high torque, normally applied in road transport vehicles and rail freight transport. The goal of a good diesel fuel, in function of its physic-chemical properties, is to promote the autoignition as fast as possible with high compression rates in order to achieve high thermal efficiency and low as possible pollutant emissions. The engine always operates at maximum volumetric efficiency, thus, what is controlled is the amount of fuel mass injected, that the bigger it is, the bigger the torque will be. However, the mass is restricted in view of a lean fuel/air mixture for maximum combustion efficiency, avoiding unburned fuel (Heywood, 1988). The diesel engine can run in a two- or four-stroke cycle. Details and a very complete explanation about the strokes for each system can be found in the literature (Heywood (1988); Martins (2013); Brunetti (2012); Merker *et al.* (2012) and references therein).

The fuel injection is done with control, in such a way that the exact amount is introduced, and also at the most appropriate angle, so that high combustion efficiency is achieved, high utilization of the work generated, smooth combustion to reduce noise, among other reasons. The quality of fuel ignition is a determining factor for compression ignition engines, which require easy ignition. It is measured by the cetane number – (CN), the property of a fuel that determines its capacity to ignite. Physically, the CN is related to the time between the start of fuel injection and the start of combustion and is called “diesel ignition delay time" (Diesel-IDT). In cases of high CN, the ignition delay is less than for fuel with low CN. The delay implies a shorter firing period, increasing the proportion of incomplete firing and, consequently, a higher specific consumption. This condition is also undesirable because it favors emissions of pollutants such as carbon monoxide (CO) and nitrogen oxides (NO_X), whose formation increases at high temperatures. Larger and more linear carbon chains, as in the case of alkanes and alkenes, have a higher CN because they are more susceptible to fragmentation by temperature, facilitating auto-ignition at lower temperatures (Brunetti, 2012; Heywood, 1988).

Note that, the fuel may have optimal physic-chemical properties for IC-ICE operation but if the piston head is not in the “optimal" configuration (as well as other engine operation/geometric characteristics) the engine could have the performance parameters and emissions affected. Rajamani *et al.* (2012) analyzed the injector characteristics and piston geometry influence on the performance parameters and emission of an ICE using the KIVA™ software. The piston bowl diameter and the arc radius of the piston bowl were then used as the main focus for analysis. In their work (Rajamani *et al.*, 2012) pointed out that bowl diameter has strong influence on the NOx and particulate matter emissions as well as in the specific fuel consumption, additionally their work shows that the arc radius of the piston bowl is relevant for NOx formation ans has less influence in the particulate matter. Kore *et al.* (2019) experimentally investigated the effect of injection pressure and piston geometry on the performance parameters of an ICE, observing the influence in the brake thermal efficiency, brake specific fuel consumption and brake power. Their results pointed our that both the investigated parameters affect the engine performance parameters. Sener and Gul (2021) report a numerical work involving CRFD using the CONVERGE™ CFD software. In their work, the piston geometry was modified (optimized), the injection angle and the start of injection (SOI) were parametrized for optimization objectives. The numerical results pointed out that optimizing the piston geometry can be reached a better diffusion combustion process as well as lower NOx and soot emissions.

3. MATERIALS AND METHODS

In order to optimize the piston head geometry of the railway ICE the AVL FIRE™ DVI tool was used. Three case studies were then performed, and described as follows:

- **Case 01**: Original case characterized using VALE S.A's internal documentation data (VALE, 2011) for General Electric's GE 7FDL engine, with 160° spray angle and original piston head geometry;
- **Case 02**: Study carried out by Henschel Jr. and Cancino (2019) characterized using VALE S.A's internal documentation data (VALE, 2011) for General Electric's GE 7FDL engine, with spray angle of 153° and original piston head geometry;
- **Case 03**: characterized using VALE SA's internal documentation data (VALE, 2011) for General Electric's GE 7FDL engine, with spray angle of 153° and piston head geometry optimized through the AVL FIRE™ DVI tool.

In the work previously carried out by Henschel Jr. and Cancino (2019) the spray dynamics was evaluated at three injection angles (160° , 153° and 167°) and according to the simulations performed, the best result was obtained for the analyzed responses using the angle of 153°. For this work, the study carried out by Henschel Jr. and Cancino (2019) is named Case 02 and the original data obtained through internal documentation of VALE S.A. (VALE, 2011) is named as Case 01. Following the work of Henschel Jr. and Cancino (2019), in this work, the optimization of the piston head geometry was performed by using the following target variables: (i) radius inside the bowl, (ii) top dead center clearance, and (iii) depth and diameter of the center of the top bowl, using the injection angle of 153°. The optimization aimed to obtain the best IMEP (indicated mean effective pressure). The optimization performed by this study is labeled as Case 03. With the results of the optimization, through numerical simulation of computational reactive fluid dynamics (CRFD), the optimized values of the piston head geometry were used and thus obtained the results in terms of power, torque, fuel consumption and emissions.

3.1 Geometric and operating parameters for simulation

The modeling was carried out using the geometric aspects of a locomotive engine based on the General Electric GE 7FDL model according to the DASH9-BB40W manual. The global geometric parameters of the modeled diesel engine are presented in Table 1. Based on studies of internal documentation of VALE S.A. (VALE, 2011), the piston geometric configuration was performed using the AVL FIRE™ ESE Diesel tool.

Table 1. GE 7FDL geometric parameters used in this work. (VALE, 2011)

Parameter	Description	Parameter	Description	Parameter	Description
Strokes	4	Stroke Length	266.7 mm	Valves	4
Cylinders	16	Compression Ratio	12.7:1	Rod Length	590.50 mm
Configuration	V	Crank Radius	133.35 mm	Piston Bore	228.6 mm

Data from Henschel Jr. and Cancino (2019)

As described in the Table 1, the engine has 16 cylinders, however the modeling was performed using only one (1) cylinder. By means of axis-symmetry condition, the combustion chamber was divided and of this form only 45° of the cylinder was modeled with only one (1) characterized fuel jet. The objective of the piston head geometry optimization was to obtain the maximum possible value of indicated mean effective pressure (IMEP). Analyzing the results obtained from the optimization, the simulation of the optimal geometric congifuration was performed, and then the results obtained in terms of power, torque, fuel consumption and emissions were then analyzed and compared to the base case.

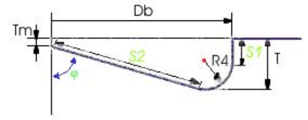
3.2 Variables for optimization

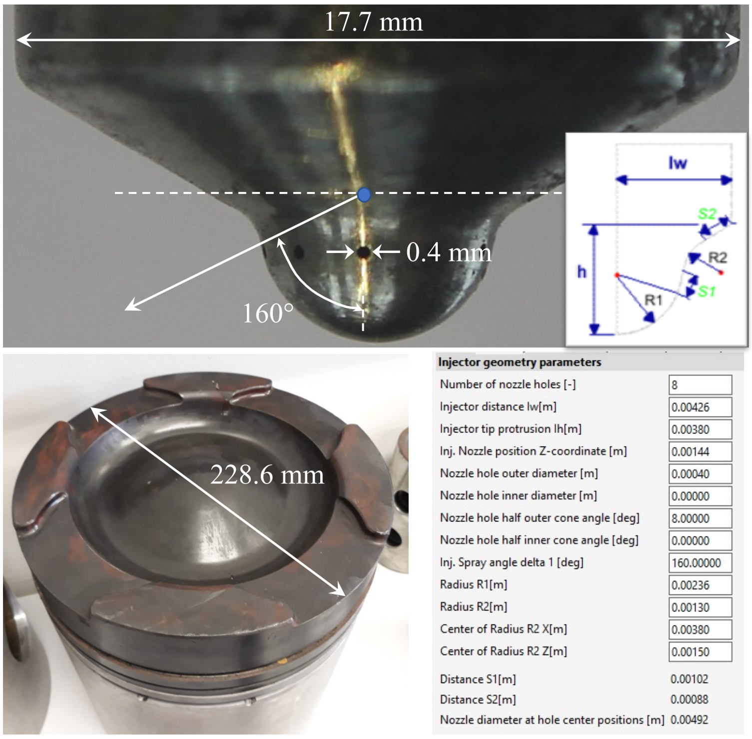
Piston head geometry optimization was performed using the AVL FIRETM DVI tool. The variables for optimization were choose based in the literature review, in a reduced number (three geometric parameters) in order to address the better expected results not allowing time- expensive computational time and resources. Table 2 shows the variables as well as the bounding adopted in this work. It is important to clarify that the even with the geometric dimension changing, the clearance volume (combustion chamber) was kept constant, not altering of this form the engine compression ratio.

3.3 Numerical model by using AVL-FIRE™

For this work, the injector and piston geometric parameters of the engine were used for simulations. Figure 1 shows the main geometric parameters of the injector and these data were kept constant for the 3 cases of this work.

Table 2. Optimization variables, lower and upper bounds

Desing Variables	**Type**	**Lower Bound**	**Base**	**Upper Bound**	**Level**	**Geometry**
R4 radius	Linear	0.009	0.18	0.027	2	
TDC Gap (Tm)	Linear	0.007675	0.01535	0.023025	2	
Bowl diameter (Db)	Linear	0.0809	0.1618	0.2427	2	
Bowl depth (T)	Linear	0.0101	0.0202	0.0303	2	



Injector geometry parameters

Number of nozzle holes [-]	8
Injector distance lw[m]	0.00426
Injector tip protrusion lh[m]	0.00380
Inj. Nozzle position Z-coordinate [m]	0.00144
Nozzle hole outer diameter [m]	0.00040
Nozzle hole inner diameter [m]	0.00000
Nozzle hole half outer cone angle [deg]	8.00000
Nozzle hole half inner cone angle [deg]	0.00000
Inj. Spray angle delta 1 [deg]	160.00000
Radius R1[m]	0.00236
Radius R2[m]	0.00130
Center of Radius R2 X[m]	0.00380
Center of Radius R2 Z[m]	0.00150
Distance S1[m]	0.00102
Distance S2[m]	0.00088
Nozzle diameter at hole center positions [m]	0.00492

Figure 1. Piston and injector geometrical parameters used in the simulations.

Figure 1 contains the values of the injector's geometric parameters used in this study. Note that the main geometric parameters of the piston and these data were kept constant in case studies 01 and 02. In case study 03, the optimization of this geometry was carried out and thus optimal values were generated which were then used in the realization of optimized simulation. Table 3 (and Fig. 1) shows the values of the piston head geometric parameters used in this work. According to Table 3, it can be seen that for cases 01 and 02 the values are based on internal documentation (VALE, 2011) and case 03 refers to the data used for the optimization of the piston head geometry obtained by through the AVL FIRE™ DVI optimization tool performed in this work.

Table 3. Piston geometric characteristics used in this work

Parameter *	Case 01	Case 02	Case 03
TDC gap [m]	0.01535	0.01535	0.01724
Db [m]	0.16180	0.16180	0.14039
T [m]	0.02020	0.02020	0.02252
Tm [m]	0.0	0.0	0.0
R4 [m]	0.01800	0.01800	0.01796
S3 [m]	0.00220	0.00220	0.00457
S2 [m]	0.06031	0.06031	0.04927
φ	71.38°	71.38°	64.98°

∗ See Fig. 1 and Table 2

Figure 2 shows the piston heads shape (and mesh) generated for simulations. Initial conditions were inserted into the model based in the previous work of Henschel Jr. and Cancino (2019) and data from (VALE, 2011). As in-cylinder operation parameters are knowledge (VALE, 2011), it was adopted strategy of not contemplating admission and exhaust strokes, os this form, the simulation begins at the closing of intake valves and finish just before the exhaust valve open, this in order to reduce computational time. Table 4 shows the initial conditions of engine at compression cycle at the best engine acceleration point (DASH9-BB40W engine), data from Henschel Jr. and Cancino (2019).

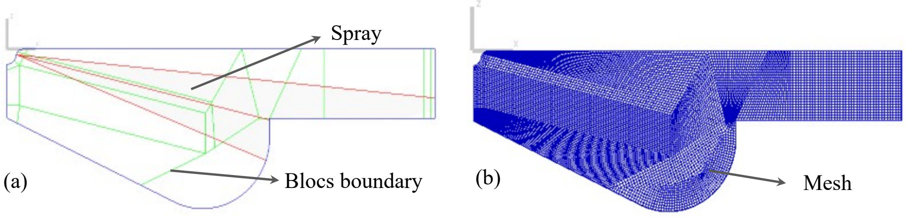


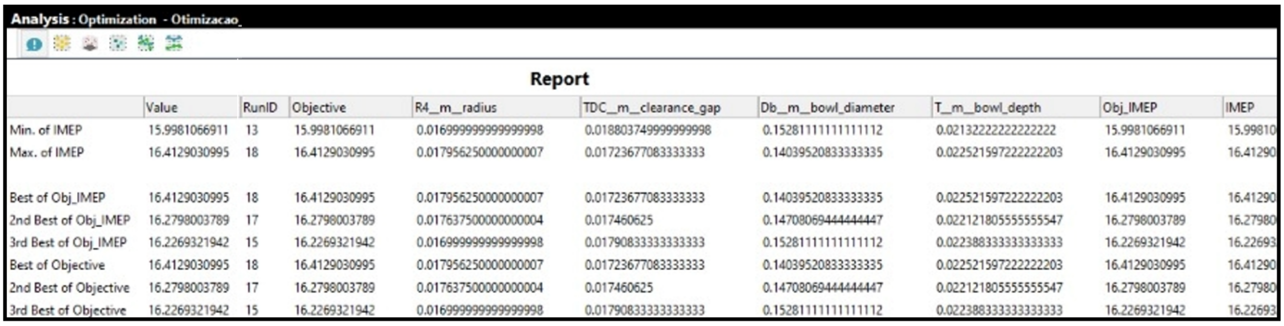
Figure 2. Combustion chamber geometry modeled at top dead center. (a) Block-structure; (b) 2D axis-symmetric mesh

Table 4. Initial conditions - DASH9-BB40W engine

Parameter	Description	Parameter	Description	Parameter	Description
Rotation [rpm]	996	Movement wall temp. [K]	570.15	EGR Mass fraction	0.049
Cylinder pressure [Pa]	255000	Fixed wall temp. [K]	470.15	Rotation direction Z	-1
Air temp. [K]	355	Fuel	Diesel-D1	Turbulent kinetic energy [m^2/s^2]	10
Fuel temp. [K]	350	Injected mass [kg]	1.10E-03	Injection duration [ms]	6.35
Swirl [1/min]	2880	Turbulent length scale [m]	0.0045	Crank angle injection start [°]	342

Data from Henschel Jr. and Cancino (2019)

The Diesel-D1 fuel from internal AVL database was used for numerical simulations. This fuel does not accurately reflect the actual fuel used because in Brazil biodiesel is added to the composition of Diesel. Turbulence, spray, transport and combustion models were used as set-up in the previous works (Henschel Jr. and Cancino, 2019; Rotter *et al.*, 2021). The moving mesh is generated using AVL FIRE FAME Engine Plus (FEP), some details of mesh parameters and dimensions are given as follows: (*i*) total number of cells = 412562 average number for all simulations along the optimization, (*ii*) number of boundary layers = 3, (*iii*) thickness of boundary layers = 0.00010 m, (*iv*) average cell size = 0.0010m with 15 subdivisions in the angular direction. Finally, the numerical simulations were performed in a computer with 8 processing cores @ 2.30 GHZ with 16 GB of RAM, a simulation that lasted approximately one week at full-time processing. Figure 3 shows the report of simulated cases in the AVL FIRE™ DVI optimization tool, along the optimization process. The values of the variables resulting from Run 18 were (see Fig. 3 - Report of optimization process) then added to the settings of a new optimized piston head geometry so that the simulation now considers this new geometry instead of the original geometry.



Report

	Value	RunID	Objective	R4__m__radius	TDC__m__clearance_gap	Db__m__bowl_diameter	T__m__bowl_depth	Obj_IMEP	IMEP
Min. of IMEP	15.9981066911	13	15.9981066911	0.016999999999999998	0.018803749999999998	0.15281111111111112	0.02132222222222222	15.9981066911	15.99810
Max. of IMEP	16.4129030995	18	16.4129030995	0.017956250000000007	0.01723677083333333	0.14039520833333335	0.022521597222222203	16.4129030995	16.41290
Best of Obj_IMEP	16.4129030995	18	16.4129030995	0.017956250000000007	0.01723677083333333	0.14039520833333335	0.022521597222222203	16.4129030995	16.41290
2nd Best of Obj_IMEP	16.2798003789	17	16.2798003789	0.017637500000000004	0.017460625	0.14708069444444447	0.022121805555555547	16.2798003789	16.27980
3rd Best of Obj_IMEP	16.2269321942	15	16.2269321942	0.016999999999999998	0.01790833333333333	0.15281111111111112	0.022388333333333333	16.2269321942	16.22693
Best of Objective	16.4129030995	18	16.4129030995	0.017956250000000007	0.01723677083333333	0.14039520833333335	0.022521597222222203	16.4129030995	16.41290
2nd Best of Objective	16.2798003789	17	16.2798003789	0.017637500000000004	0.017460625	0.14708069444444447	0.022121805555555547	16.2798003789	16.27980
3rd Best of Objective	16.2269321942	15	16.2269321942	0.016999999999999998	0.01790833333333333	0.15281111111111112	0.022388333333333333	16.2269321942	16.22693

Figure 3. Report of optimization process

4. RESULTS

The optimization of the piston head geometry changed the characterization of the combustion process. The combustion of 90% of the mixture for case 03 was anticipated on average by 5.22° , going from 761.68° on average to 756.46° as can be seen in Table 5 and Fig. 4. Nevertheless, the most notable difference regards the combustion duration. For Case 03 (optimized one) the combustion duration (10% to 90%) is the shortest one, indicating that combustion process is faster for the optimized piston head geometry.

Table 5. Combustion characterization

Mass Burned Fraction	**Case 01** (°CA)	**Case 02** (°CA)	**Case 03** (°CA)		**Combustion Duration** (°CA)	**Case 01** (°CA)	**Case 02** (°CA)	**Case 03** (°CA)
2%	709.12	709.2	709.38		2% - 90%	52.93	52.11	47.08
10%	710.24	710.37	710.59		10% - 50%	1.54	1.48	1.53
50%	711.79	711.85	712.13		10% - 90%	51.81	50.93	45.87
90%	762.06	761.31	756.46					

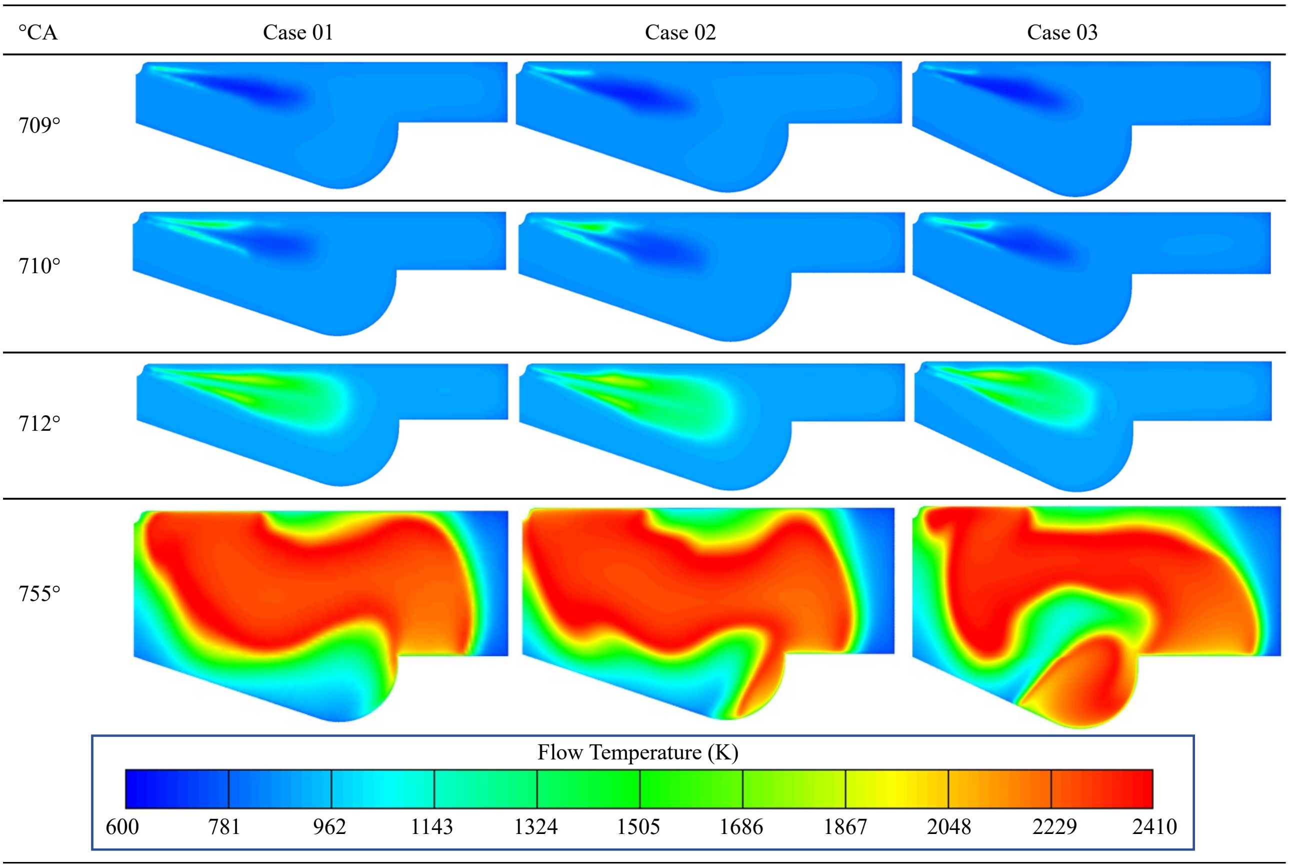


Figure 4. Flow temperature for all cases investigated in this work - Case 03 is the best geometric configuration pointed out by the AVL FIRE™ DVI optimization tool

In addition, the optimization of the piston head geometry generated a slight increase in the average temperature as well as a small displacement of this temperature in relation to the crank angle, as can be seen in Fig. 5. This way, the optimized case keeps a higher temperature levels for longer, and this might be related to the faster combustion duration.

4.1 Emissions

Figure 5 also shows that higher temperatures are reached for the optimized geometry (case 03) around the top dead center, the higher the temperature the higher the pressure and the higher the chance of NOx chemistry activation as observed in Fig. 6(a). Therefore, despite having the best IMEP and power output, the optimized case had its NO_X levels increased probably due to the longer exposition to higher temperatures. The effect of in-cylinder temperature increase can explain the emission behavior in the optimized piston head geometry. Usually higher values of power and torque are followed by increase in emissions related to higher temperatures, of this form, the after-treatment gases system are usually adapted in order to overcome the issue (bare in mind that this aspect is beyond the scope of this work).

Regarding carbon-related emissions, Fig. 6 (b) to (d) shows soot, CO_2 and CO mean mass fractions. Note that the optimized case produced higher CO_2 emissions. However, this does not seem an issue, since soot and CO levels were lower. In other words, more CO_2 reflects an overall more complete combustion process, as the intermediate and less-oxidized carbon products simultaneously decrease.

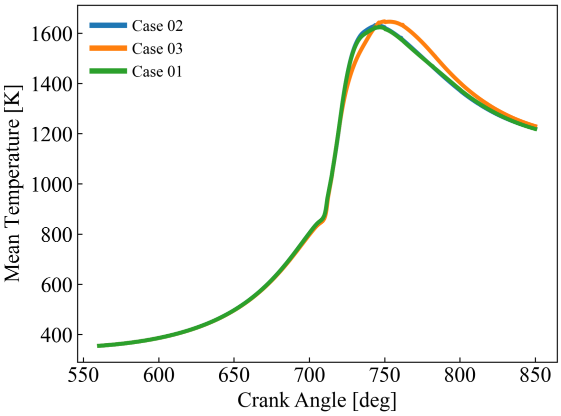


Figure 5. In cylinder temperature calculated for all the cases investigated in this work

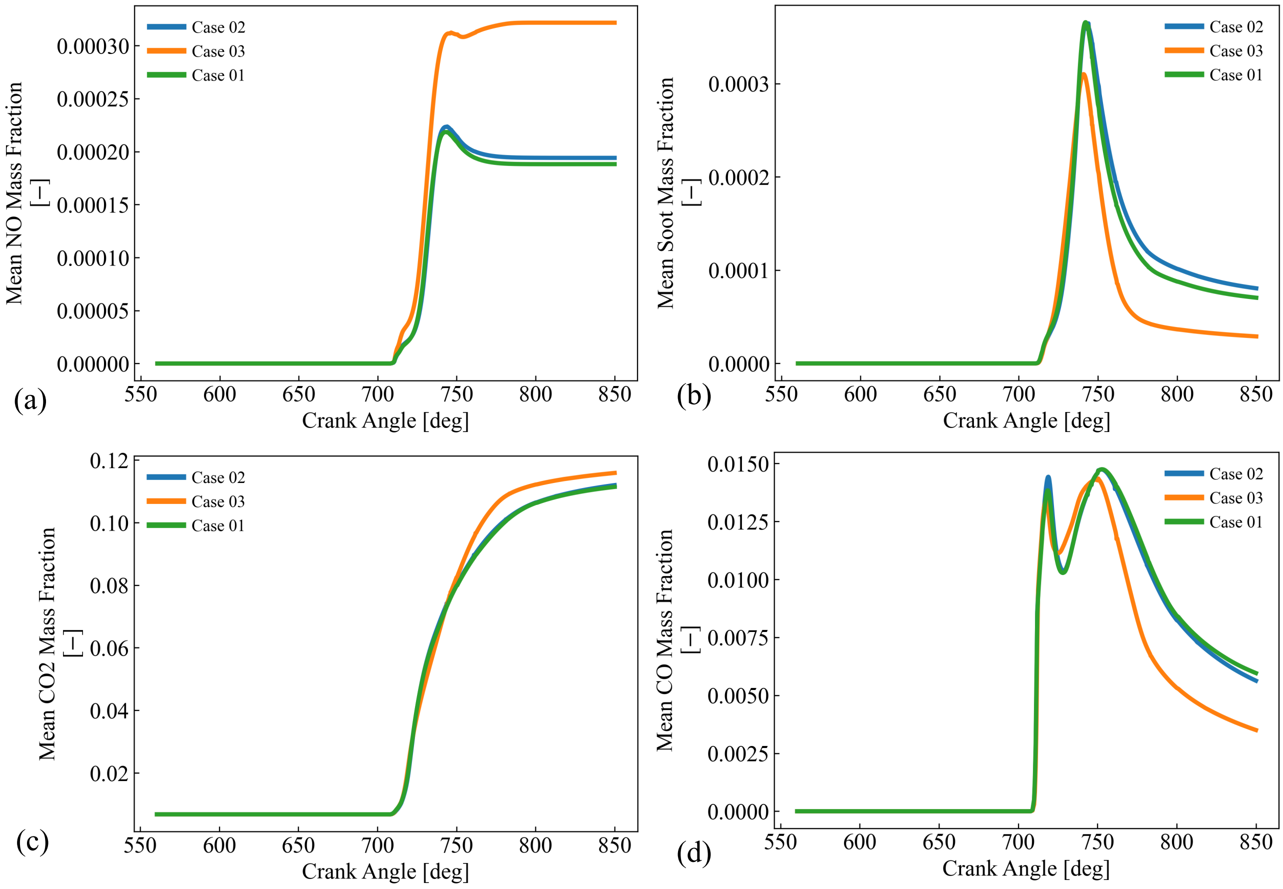


Figure 6. Calculated emissions for all the cases investigated in this work. (a) NO mass fraction. (b) Soot mass fraction. (c) CO2 mass fraction. (d) CO mass fraction

4.2 Engine performance parameters - Improvements from optimization process

The results of the simulations performed in this work are described in Table 6. It can be seen that there was a gain referring to the change in the injection angle from 160° to 153° as verified in the comparisons between cases 01 and 02. However, when we optimize the geometry of the piston head, this gain is enhanced as can be seen in the comparison between cases 01 and 03. The optimization of the piston head geometry resulted in obtaining a 2.88% higher IMEP compared to case 01, in the same way there was a gain in power and indicated torque of 2.18%. When evaluating the indicated thermal efficiency, this gain was 2.63%. There was also a reduction in the specific fuel consumption indicated in the order of 2.78%. Please note that, Table 6 shows the improvements on engine performance parameters obtained in the work of Henschel Jr. and Cancino (2019) (Case 01 to Case 02) and the improvements obtained from the geometric piston head optimization process performed in this work (Case 01 to Case 03).

Table 6. Relative improvement of the Case 03 (the optimized one)

Case	**Mean Effective Pressure** (bar)	**Indicated Power** (kW)	**Indicated Torque** (N.m)	**Air-fuel ratio (λ)** (–)	**Indicated Specific Fuel Consumption** (kg/kW.h)	**Indicated Thermal Efficiency** (–)
Case 01	15.95	145.94	1399.25	1.77	0.2269	0.38
Case 02	16.00	146.33	1402.92	1.77	0.2263	0.38
Improvement † Case 01 to Case 02	0.31%	0.27%	0.26%	0.0%	-0.26%	0.0%
Case 03	16.41	149.12	1429.69	1.77	0.2206	0.39
Improvement ‡ Case 01 to Case 03	2.88%	2.18%	2.18%	0.0%	-2.78%	2.63%

† related to the work of Henschel Jr. and Cancino (2019)

‡ obtained in this work

5. CONCLUSSION

The simulation results indicate that the piston head optimization generated a considerable gain in terms of engine power and torque, as well as a reduction in the specific fuel consumption. Regarding emissions, the level of soot emitted was reduced, however there was a slight increase in the emission of CO2 and considerable increase of NO, regarding the higher temperature observed in the optimized geometry (Case 03, in Fig. 5). It is observed that the simulation did not take into account the recirculation of gases through EGR, which can be a determining factor for the reduction of emissions. Still with regard to the injection angle, it was considered to use the angle of 153° , giving a segment to the study carried out by Henschel Jr. and Cancino (2019). Which had already shown a slight improvement in results in terms of power and torque. It is also noted that the characterization of the combustion was changed due to the optimization of the piston head geometry as the combustion of 90% of the mixture was anticipated on average by 5.22° CA. The average temperature obtained was slightly higher when the simulation used the optimized piston head geometry, thus justifying the slight increase in production and NO and CO2. The results obtained with the simulations indicate that the optimization of the piston head geometry can represent a considerable gain in terms of power and torque in a real engine model DASH9-BB40W, and that this optimization can also represent a reduction in fuel consumption, for that, new studies in order to add the recirculation of gases through EGR in order to reduce the emission of NO and CO2 are necessary. It is noteworthy that this work has the exclusive purpose of studies and does not represent an indication of use as it is an exploratory study.

6. ACKNOWLEDGEMENTS

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